

2,4,8,10-Tetraoxaspiro[5.5]undecane
126-54-5 | DTXSID2059566

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 212 °C

Global applicability domain: Inside

Local applicability domain index: 6.12e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl 2,2-dichloroacetoacetate

Measured: 206

Predicted: 210

Image not found

2-Chloroethyl acetoacetate

Measured: 198

Predicted: 199

Image not found

4-Octanolide

Measured: 234

Predicted: 216